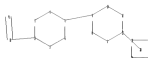
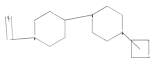


10/540304

=>

Uploading C:\Documents and Settings\EBernhardt\My
Documents\Stnexp\Queries\10540304.str



chain nodes :

13 14

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 16 17 18 19

chain bonds :

2-13 5-9 13-14

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 16-17 16-19

17-18 18-19

exact/norm bonds :

1-2 1-6 2-3 2-13 3-4 4-5 5-6 5-9 7-8 7-12 8-9 9-10 10-11 11-12 13-14

16-17 16-19 17-18 18-19

isolated ring systems :

containing 1 : 7 :

G1:O,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom

11:Atom 12:Atom 13:CLASS 14:CLASS 16:Atom 17:Atom 18:Atom 19:Atom 20:CLASS

10/540304

L1 STRUCTURE UPLOADED

=> s l1

SAMPLE SEARCH INITIATED 14:03:51 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 1802 TO ITERATE

100.0% PROCESSED 1802 ITERATIONS

1 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 33494 TO 38586

PROJECTED ANSWERS: 1 TO 80

L2 1 SEA SSS SAM L1

=> s l1 sss full

FULL SEARCH INITIATED 14:03:57 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 34077 TO ITERATE

100.0% PROCESSED 34077 ITERATIONS

22 ANSWERS

SEARCH TIME: 00.00.01

L3 22 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

172.10

172.31

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FILE COVERS 1907 - 26 Dec 2007 VOL 147 ISS 26

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=> s l3

L4 1 L3

=> d 14 bib abs hitstr

L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN
 AN 2004:550949 CAPLUS
 DN 141:106497
 TI Preparation of substituted 1-piperidin-4-yl-4-azetidin-3-yl-piperazine
 derivatives and their use as neurokinin antagonists
 IN Janssens, Frans Eduard; Sommen, Francois Maria; De Boeck, Benoit Christian
 Albert Ghislain; Leenaerts, Joseph Elisabeth
 PA Janssen Pharmaceutica N.V., Belg.
 SO PCT Int. Appl., 52 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004056800	A1	20040708	WO 2003-EP51042	20031217
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SV, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	CA 2509406	A1	20040708	CA 2003-2509406	20031217
	AU 2003299249	A1	20040714	AU 2003-299249	20031217
	EP 1581517	A1	20051005	EP 2003-799583	20031217
	EP 1581517	B1	20070221		
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	JP 2006512349	T	20060413	JP 2004-561505	20031217
	AT 354572	T	20070315	AT 2003-799583	20031217
	ES 2282731	T3	20071016	ES 2003-3799583	20031217
	US 2006074069	A1	20060406	US 2005-540304	20050621
PRAI	WO 2002-EP14837	A	20021223		
	WO 2003-EP51042	W	20031217		
OS	MARPAT 141:106497				
GI					

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. I [Q = O or NR3; X = covalent bond, -O-, -S-, or -NR3; R1 independently = Ar1, Ar1-alkyl, and di(Ar1)-alkyl; R2 = Ar2, Ar2-alkyl, di(Ar2)-alkyl Het1, Het1-alkyl; R3 independently = H or alkyl; Y = covalent bond, -CO-, -SO2-, >C=CHR or >C=NR, wherein R = H, CN or NO2; M independently = covalent bond, (un)substituted-alkyl, -(un)saturated carbocycle; L = H, alkyloxy, Ar3oxy, alkylamine, etc.; Ar1 = (un)substituted phenyl; Ar2 = (un)substituted naphthalenyl or Ph with substituent(s) selected from halo, alkyl, CN, aminocarbonyl, and alkyloxy; Ar3 = (un)substituted naphthalenyl or Ph with substituent(s) selected from

halo, alkyl, CN, amino, alkyloxy, OH, pyridinyl, etc.; Het1 = monocyclic heterocyclic radical selected from pyrrolyl, pyrazolyl, imidazolyl, furanyl, etc.; m = 1 or 2 provided that if m = 2, then n = 1; n = 0-2; p = 1-2; q = 0-1 and their pharmaceutically acceptable salts having neurokinin antagonistic activity, in particular NK1 antagonistic activity and NK1/NK3- antagonistic activity, their preparation, compns. comprising them and their use as a medicine, in particular for the treatment of schizophrenia, emesis, anxiety, depression, irritable bowel syndrome (IBS), circadian rhythm disturbances, pain, neurogenic inflammation, asthma, micturition disorders such as urinary incontinence and nociception are disclosed. Thus, e.g., II was prepared by reaction of (2R-trans)-1-[3,5-bis(trifluoromethyl)benzoyl]-2-(phenylmethyl)-4-(1-piperazinyl)piperidine (preparation given) with 1-(diphenylmethyl)-3-azetidiny methanesulfonate. For selected compds. of the invention, receptor binding pIC50 values for h-NK1 were in a range from 6.69-8.13. In view of their capability to antagonize the actions of tachykinins by blocking the neurokinin receptors, and in particular antagonizing the actions of substance P by blocking the NK receptors, the compds. according to the invention are useful as a medicine, in particular in the prophylactic and therapeutic treatment of tachykinin mediated conditions, such as, for instance CNS disorders, in particular depression, anxiety disorders, stress-related disorders, sleep disorders, cognitive disorders, personality disorders, schizoaffective disorders, eating disorders, neurodegenerative diseases, addiction disorders, mood disorders, sexual dysfunction, pain and other CNS related conditions; inflammation; allergic disorders; emesis; gastrointestinal disorders, in particular irritable bowel syndrome (IBS); skin disorders; vasospastic diseases; fibrosing and collagen diseases; disorders related to immune enhancement or suppression and rheumatic diseases and body weight control.

IT 718637-71-9P 718637-72-0P 718637-73-1P
718637-74-2P 718637-75-3P 718637-76-4P
718637-77-5P 718637-78-6P 718637-79-7P
718637-80-0P 718637-81-1P 718637-82-2P
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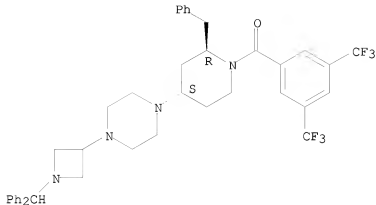
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(stereoselective preparation of piperidylazetidiny piperazines with tachykinin antagonist activity)

RN 718637-71-9 CAPLUS

CN Piperidine, 1-[3,5-bis(trifluoromethyl)benzoyl]-4-[4-[1-(diphenylmethyl)-3-azetidiny]-1-piperazinyl]-2-(phenylmethyl)-, (2R,4S)- (9CI) (CA INDEX NAME)

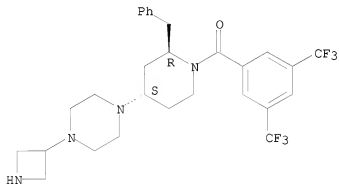
Absolute stereochemistry.



RN 718637-72-0 CAPLUS

CN Piperidine, 4-[4-(3-azetidinyl)-1-piperazinyl]-1-[3,5-bis(trifluoromethyl)benzoyl]-2-(phenylmethyl)-, (2R,4S)- (9CI) (CA INDEX NAME)

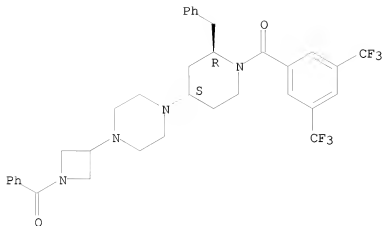
Absolute stereochemistry.



RN 718637-73-1 CAPLUS

CN Piperidine, 4-[4-[(1-benzoyl-3-azetidinyl)-1-piperazinyl]-1-piperidinyl]-1-[3,5-bis(trifluoromethyl)benzoyl]-2-(phenylmethyl)-, (2R,4S)- (9CI) (CA INDEX NAME)

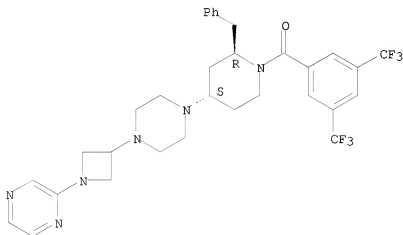
Absolute stereochemistry.



RN 718637-74-2 CAPLUS

CN Piperidine, 1-[3,5-bis(trifluoromethyl)benzoyl]-2-(phenylmethyl)-4-[4-(1-pyrazinyl-3-azetidyl)-1-piperazinyl]-, (2R,4S)- (9CI) (CA INDEX NAME)

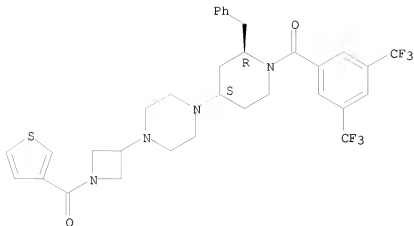
Absolute stereochemistry.



RN 718637-75-3 CAPLUS

CN Piperidine, 1-[3,5-bis(trifluoromethyl)benzoyl]-2-(phenylmethyl)-4-[4-[1-(3-thienylcarbonyl)-3-azetidyl]-1-piperazinyl]-, (2R,4S)- (9CI) (CA INDEX NAME)

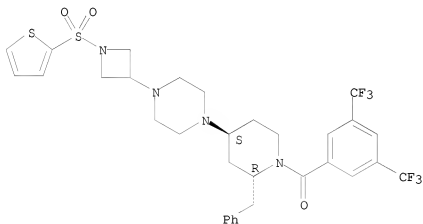
Absolute stereochemistry.



RN 718637-76-4 CAPLUS

CN Piperidine, 1-[3,5-bis(trifluoromethyl)benzoyl]-2-(phenylmethyl)-4-[4-[1-(2-thienylsulfonyl)-3-azetidiny]-1-piperazinyl]-, (2R,4S)- (9CI) (CA INDEX NAME)

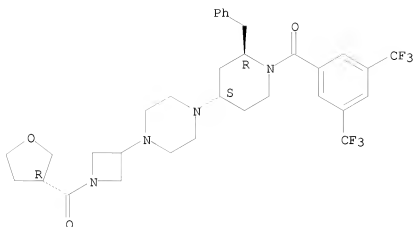
Absolute stereochemistry.



RN 718637-77-5 CAPLUS

CN Piperidine, 1-[3,5-bis(trifluoromethyl)benzoyl]-2-(phenylmethyl)-4-[4-[1-[(3R)-tetrahydro-3-furanyl]carbonyl]-3-azetidiny]-1-piperazinyl]-, (2R,4S)- (9CI) (CA INDEX NAME)

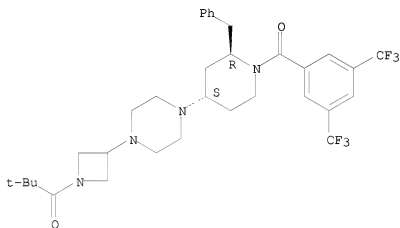
Absolute stereochemistry.



RN 718637-78-6 CAPLUS

CN Piperidine, 1-[3,5-bis(trifluoromethyl)benzoyl]-4-[4-[1-(2,2-dimethyl-1-oxopropyl)-3-azetidiny]-1-piperazinyl]-2-(phenylmethyl)-, (2R,4S)- (9CI) (CA INDEX NAME)

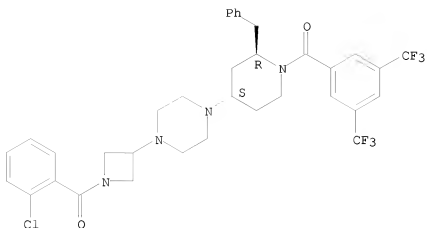
Absolute stereochemistry.



RN 718637-79-7 CAPLUS

CN Piperidine, 1-[3,5-bis(trifluoromethyl)benzoyl]-4-[4-[1-(2-chlorobenzoyl)-3-azetidiny]-1-piperazinyl]-2-(phenylmethyl)-, (2R,4S)- (9CI) (CA INDEX NAME)

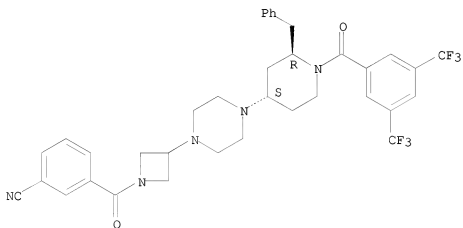
Absolute stereochemistry.



RN 718637-80-0 CAPLUS

CN Piperidine, 1-[3,5-bis(trifluoromethyl)benzoyl]-4-[4-[1-(3-cyanobenzoyl)-3-azetidiny]-1-piperazinyl]-2-(phenylmethyl)-, (2R,4S)- (9CI) (CA INDEX NAME)

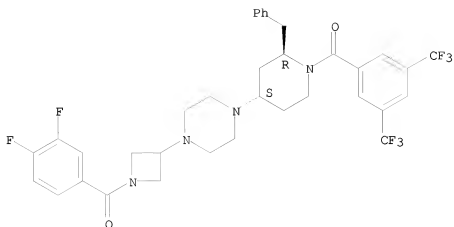
Absolute stereochemistry.



RN 718637-81-1 CAPLUS

CN Piperidine, 1-[3,5-bis(trifluoromethyl)benzoyl]-4-[4-[1-(3,4-difluorobenzoyl)-3-azetidiny]-1-piperazinyl]-2-(phenylmethyl)-, (2R,4S)- (9CI) (CA INDEX NAME)

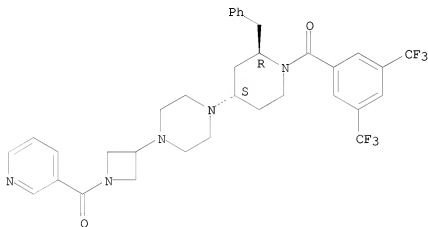
Absolute stereochemistry.



RN 718637-82-2 CAPLUS

CN Piperidine, 1-[3,5-bis(trifluoromethyl)benzoyl]-2-(phenylmethyl)-4-[4-[1-(3-pyridinylcarbonyl)-3-azetidinyl]-1-piperazinyl]-, (2R,4S)- (9CI) (CA INDEX NAME)

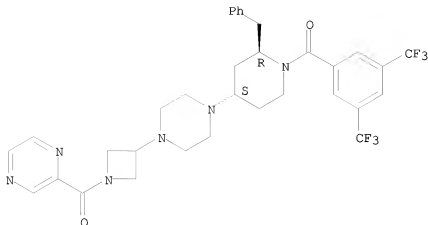
Absolute stereochemistry.



RN 718637-83-3 CAPLUS

CN Piperidine, 1-[3,5-bis(trifluoromethyl)benzoyl]-2-(phenylmethyl)-4-[4-[1-(pyrazinylcarbonyl)-3-azetidinyl]-1-piperazinyl]-, (2R,4S)- (9CI) (CA INDEX NAME)

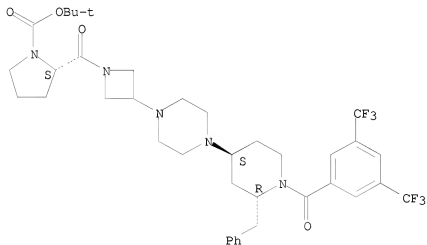
Absolute stereochemistry.



RN 718637-84-4 CAPLUS

CN 1-Pyrrolidinecarboxylic acid, 2-[[[3-[4-[(2R,4S)-1-[3,5-bis(trifluoromethyl)benzoyl]-2-(phenylmethyl)-4-piperidinyl]-1-piperazinyl]-1-azetidiny]carbonyl]-, 1,1-dimethylethyl ester, (2S)- (CA INDEX NAME)

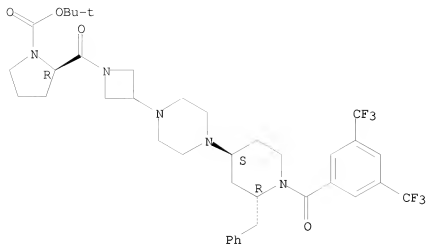
Absolute stereochemistry.



RN 718637-85-5 CAPLUS

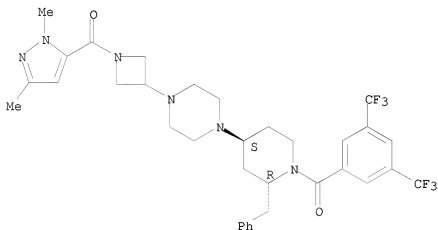
CN 1-Pyrrolidinecarboxylic acid, 2-[[[3-[4-[(2R,4S)-1-[3,5-bis(trifluoromethyl)benzoyl]-2-(phenylmethyl)-4-piperidinyl]-1-piperazinyl]-1-azetidiny]carbonyl]-, 1,1-dimethylethyl ester, (2R)- (CA INDEX NAME)

Absolute stereochemistry.



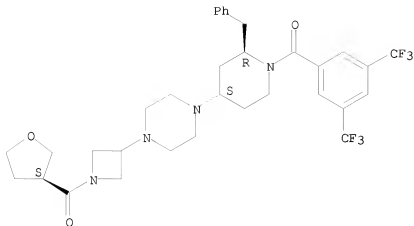
RN 718637-86-6 CAPLUS
 CN Piperidine, 1-[3,5-bis(trifluoromethyl)benzoyl]-4-[4-[1-[(1,3-dimethyl-1H-pyrazol-5-yl)carbonyl]-3-azetidinyl]-1-piperazinyl]-2-(phenylmethyl)-, (2R,4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 718637-87-7 CAPLUS
 CN Piperidine, 1-[3,5-bis(trifluoromethyl)benzoyl]-2-(phenylmethyl)-4-[4-[1-[[[(3S)-tetrahydro-3-furanyl]carbonyl]-3-azetidinyl]-1-piperazinyl]-, (2R,4S)- (9CI) (CA INDEX NAME)

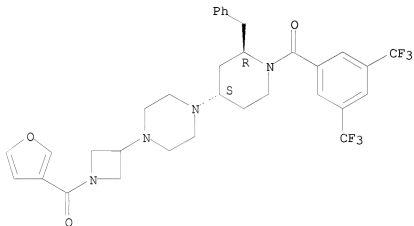
Absolute stereochemistry.



RN 718637-88-8 CAPLUS

CN Piperidine, 1-[3,5-bis(trifluoromethyl)benzoyl]-4-[4-[1-(3-furanylcarbonyl)-3-azetidinyl]-1-piperazinyl]-2-(phenylmethyl)-, (2R,4S)-(9CI) (CA INDEX NAME)

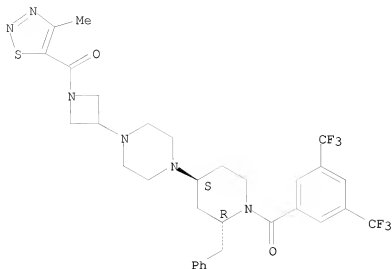
Absolute stereochemistry.



RN 718637-89-9 CAPLUS

CN Piperidine, 1-[3,5-bis(trifluoromethyl)benzoyl]-4-[4-[1-[(4-methyl-1,2,3-thiadiazol-5-yl)carbonyl]-3-azetidinyl]-1-piperazinyl]-2-(phenylmethyl)-, (2R,4S)-(9CI) (CA INDEX NAME)

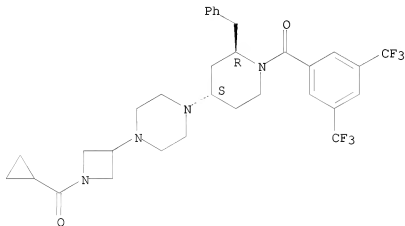
Absolute stereochemistry.



RN 718637-90-2 CAPLUS

CN Piperidine, 1-[3,5-bis(trifluoromethyl)benzoyl]-4-[4-[1-(cyclopropylcarbonyl)-3-azetidyl]-1-piperazinyl]-2-(phenylmethyl)-, (2R,4S)- (9CI) (CA INDEX NAME)

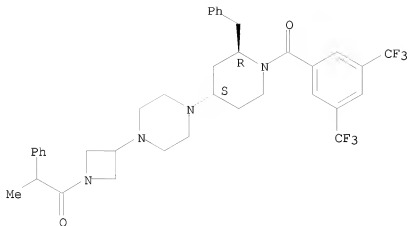
Absolute stereochemistry.



RN 718637-91-3 CAPLUS

CN Piperidine, 1-[3,5-bis(trifluoromethyl)benzoyl]-4-[4-[1-(1-oxo-2-phenylpropyl)-3-azetidyl]-1-piperazinyl]-2-(phenylmethyl)-, (2R,4S)- (9CI) (CA INDEX NAME)

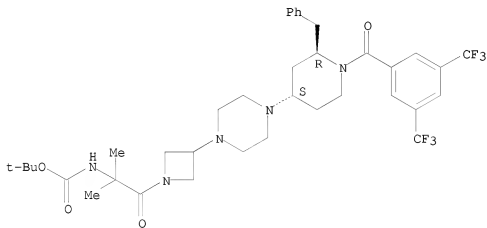
Absolute stereochemistry.



RN 718637-92-4 CAPLUS

CN Carbamic acid, [2-[3-[4-[(2R,4S)-1-[3,5-bis(trifluoromethyl)benzoyl]-2-(phenylmethyl)-4-piperidinyl]-1-piperazinyl]-1-azetidiny]-1,1-dimethyl-2-oxoethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
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L5 0 L3

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10/540304

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L6 0 L3

=> log h

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TOTAL

ENTRY

SESSION

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SINCE FILE

TOTAL

ENTRY

SESSION

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